Quantification of Information from Lattice Images: Local Lattice Parameters and Chemical Composition

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NCEM provides sophisticated image analysis software that enables scientists to extract quantitative information about the local composition and structure of materials from lattice images. Recently, it was shown that local displacements as small as 1 pm can be detected in systems with low crystallographic symmetry at a spatial resolution of 0.3-0.5 nm. The developed method was applied to analyze the light emission from commercialized GaN/InGaN/AlGaN heterostructures.

Background – A lattice image from an electron microscope holds encoded information about the structure, the chemical composition and the thickness of the investigated samples. This information is stored in form of an image that can be digitized as an array of gray levels. 10^6 bits of information are stored in a 1k x 1k image. Computer science enables scientists to "mine" this huge amount of data for the desired information that may be of chemical [1,2] or of structural nature [3]. For example, the determination of local lattice parameters from a lattice image is typical for the type of information that scientists seek to know.

Accomplishment - NCEM develops and provides software that enables researchers to determine the size of projected unit cells from a digitized lattice image with sub-pixel accuracy. Unit cells of lattice images are related to the material's lattice constants which, therefore, can be determined and mapped. Unlike other implementations of this idea, the software at NCEM can be applied to systems of cubic and lower symmetry. It was demonstrated that local displacements in hexagonal GaN of 1 pm can be measured with a lateral resolution of 0.3-0.5 nm [3].

Figure 1 shows a pseudomorphically grown $Al_xGa_{1-x}N$ barrier layer in GaN deposited by Metal Organic Chemical Vapor Deposition (MOCVD) to test the procedure. Lattice imaging (a) was performed with the Atomic Resolution Microscope. The 800keV electrons of the instrument penetrate foils that are thicker than usual. Thereby, stress relaxation effects can be minimized. Figure 1b compares composition profiles across the structure obtained by K_{Al} electron energy loss and by local measurements of lattice parameters. It is seen that the resulting strain across the structure closely follows the local Al composition. The effect is caused by the smaller size of the Al atom compared with Ga. The lattice parameters and/or the resulting local strain can be mapped at a lateral resolution of 0.5 – 0.3 nm (figure 1c).

Figure 2 shows an application. Strain profiles across the active region of commercially available n-GaN/InGaN/AlGaN/p-GaN green and blue Light Emitting Diodes are shown. Such structures currently revolutionize the lighting industry. It was speculated that the shift of the light emission from blue to green is caused by an increased In content. However, it is seen in figure 2 that the In as well as the Al concentration concentrations are not significantly different because the strain is identical within errors. Instead, it is the InGaN well width that is reduced to shift the light emission from green to blue.

The ability to map lattice parameters with an accuracy of 1pm at a lateral resolution of 0.3–0.5 nm in systems of cubic or lower symmetry is expected to become an important tool for the quantitative analysis of materials.

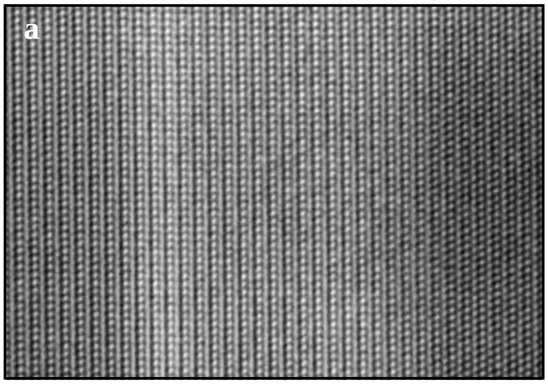
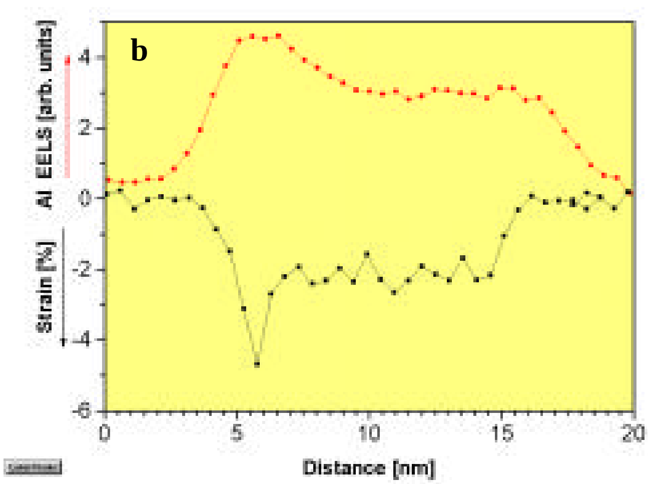
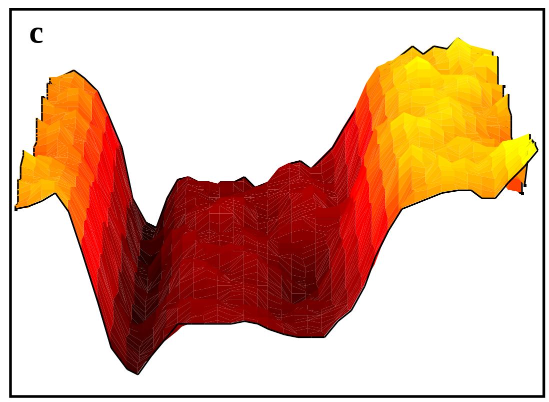


Figure 1:
a) Lattice image of a $GaN/Al_xGa_{1-x}N/GaN$ quantum well.
b) Comparison of the Al profile across the quantum well recorded by electron energy loss spectroscopy (EELS) with the measured strain profile.
c) Three dimensional map of the lattice constant.





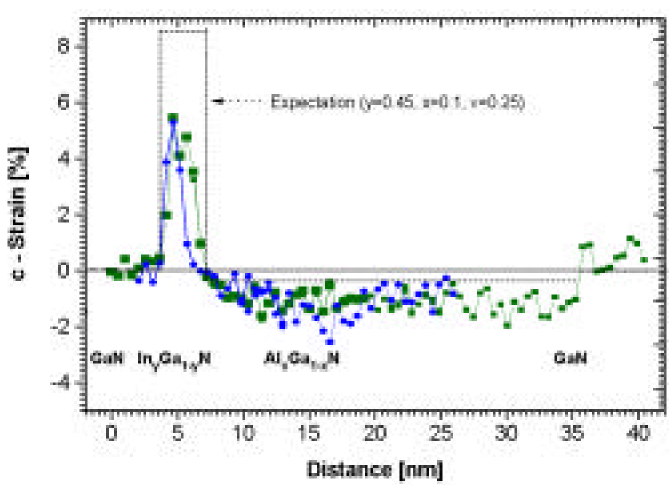


Figure 2: Strain profiles across the active region of green (green squares) and blue (blue circles) LED's. The strain is proportional to the impurity content (In, Al). Dashed line represents speculations from literature. Quantitative analysis reveals that the blue shifted light emission stems from a reduction of the InGaN well width to 1.5 nm.

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